

The metal-insulator transition in semiconductors

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(Dated: February 25, 2009)

Abstract

The temperature dependence of the number density of elementary excitations in a semiconductor with account for the temperature dependence of the band gap is obtained. A local lattice distortion within a crystalline domain is discussed.

PACS numbers: 71.30.+h, 71.20.-b

Recently, it was shown [1] that there is a general relation between the band gap E_g at zero temperature $T = 0K$ and the metal-insulator transition temperature T_{MI} of the form

$$E_g = \alpha k_B T_{MI}, \quad (1)$$

where k_B is the Boltzmann constant and $\alpha \approx 18$.

The temperature dependence of the band gap is given by the equation

$$E_g(T) = E_g - \beta k_B T, \quad (2)$$

where the value of the constant β is normally close to 6 ($\beta = 6$ in the case of ZnS and $\beta = 5$ in the case of Si, Ge, and GaAs).

The relation (2) modifies the temperature dependence of the number density n of elementary excitations [1] in a semiconductor as follows

$$n = n_0 (T_{MI}/T)^{\beta+1} \exp(-E_g/k_B T), \quad (3)$$

where $n_0 \approx 1.1 \times 10^{22} \text{cm}^{-3}$ is a constant. At the transition temperature $T = T_{MI}$, the equations (3) and (1) give the critical number density of elementary excitations,

$$n_c = n_0 \exp(-\alpha) = d_c^{-3}, \quad (4)$$

where $d_c \approx 180 \text{nm}$ is the size of the region around a point defect in a semiconductor within which there is a local lattice distortion of a ferroelastic type [2] caused by the charge redistribution. The amplitude $\delta = \Delta a/a$ (a is the lattice parameter) of this local lattice distortion has an order of 10^{-4} [2]. There is also a general ferroelastic lattice distortion associated with the metal-insulator transition [2] the amplitude of which is much higher, $\delta \cong 10^{-2}$.

The energy of an elementary excitation in a semiconductor is equal to the band gap E_g . For semiconductors with similar chemical compositions, there is a relation between the band gap at zero temperature and the energy E_v of the vacancy formation which is given by the equation similar to the equation (1),

$$E_v = \alpha k_B T_m, \quad (5)$$

where T_m is the melting temperature. For cadmium chalcogenides, the ratio E_g/E_v is $E_g/E_v \approx 0.8$. For zinc chalcogenides, this ratio is $E_g/E_v \approx 1.15$. In GaAs and GaSb, the band gap is $E_g \approx 0.6E_v$.

[1] F.V.Prigara, arXiv:0805.4325 (2008).

[2] F.V.Prigara, arXiv:0811.1131 (2008).

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